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EXPERIMENTAL AND THEORETICAL INVESTIGATIONS OF ANTI-CORROSIVE PROPERTIES OF THYMOL

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Abstract. The inhibition effect of thymol during the early stage of steel corrosion under adsorbed thin electrolyte layers was investigated. Its vapor corrosion inhibition property was evaluated under simulated operational conditions. Electrochemical techniques complemented by FTIR and SEM surface analyses were used to evaluate the composition and characteristics of the layers. The results indicate that thymol can form a protective film on the metal surface, which protects the metal against further corrosion. Quantum chemical calculations studies were also performed to support weight loss and electrochemical experimental observations.

Keywords: atmospheric corrosion, thymol, steel, volatile inhibitor, quantum chemical calculations.

1. Introduction

Temporary corrosion protection is designed to prevent the corrosion of metal surfaces of equipment during transportation and storage [1-4]. There are many types of temporary protection methods. Among them, the use of volatile corrosion inhibitors (VCI) is an effective and convenient means. There are numerous investigations on aliphatic amines, alicyclic amines, and their salts as VCI for corrosion inhibitions of various industrial metals and alloys, but some of these inhibitors are toxic, expensive and non-biodegradable. However, as a result of their high cost and increasing awareness of health and ecological risks, attention is being drawn towards finding highly efficient, cheaper and non-toxic inhibitors. The present trend in research on environmental friendly corrosion inhibitors is concentrating on products of natural origin due principally to their low cost and eco-friendliness [5-10].

Thus, it was shown that the wastes of the production of oil from rapeseeds (*Brassicaceae* family) [6, 7], hop cones (*Humulus lupulus* family), pomaces of grapes (*Vitis vinifera* family) [8], wood bark oil [9], and thyme [10, 11] can be a source of natural organic compounds for the preparation of VCI. The plant extract is a mixture of various components, which results in the complex inhibitive mechanism. It is rather difficult to determine what components present in plant extract create their relatively high ability to inhibit corrosion. A better way is to isolate the components and investigate the inhibition of each single component, but it is still difficult to isolate all the components. Thus, testing the inhibition potential of major components using available pure compounds could be an alternative choice to study the corrosion inhibition of plant extract. Through these studies, it is agreed that the inhibition performance of plant extract is normally ascribed to the presence in their composition of complex organic species such as aldehydes, terpenoids, glycosides, nucleosides, ketones and aldehydes, saturated and unsaturated fatty acids. The inhibition of mild steel corrosion by the studied species of plant raw materials [6, 7-11] is probably attributed to the presence of most important compounds such as monoterpenoid phenol – thymol (2-isopropyl-5-methylphenol). Hence, the objective of this study was to investigate the inhibitory effect of thymol as green volatile corrosion inhibitor mild steel.

2. Experimental

2.1. Materials and Apparatus

The corrosion test and electrochemical measurements were carried out using mild steel strips. The composition of the mild steel is given in wt %: C 0.21; Mn 0.05; P 0.09; S 0.05 and 0.01 Al; P 0.02 at all Fe. Before research, samples of St3 were sandwiched with different grains (0.1, 2/0, 3/0), degreased and kept in a desiccator for 1 day. The inhibitor used was thymol with the concentration range from 50 to 600 mg/l. Fig. 1 shows the molecular structure of thymol.

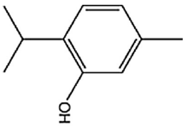

Fig. 1. The molecular structure of thymol

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2.2. Gravimetric Measurements

The gravimetric tests were carried out according to the JB/T 6071 standard with a few modifications. The final geometrical area was 25 cm^2. Each test was done with three specimens at the same time to give reproducible results. The test process included cyclic warming and cooling of the samples in a corrosion testing chamber of varying humidity. One cycle included 8 h exposure in the thermostat (313 ± 1 K), and 16 h exposure at room temperature of 298 K). The total duration of the tests was 21 days. The efficiency of inhibitors was estimated according to the degree of protection against corrosion (IE) [7, 8].

2.3. Electrochemical Measurements

Electrochemical experiments were carried out in a conventional three-electrode cell with a platinum counter electrode (CE) and a saturated calomel electrode (SCE) coupled to a fine Luggin capillary as the reference electrode. An electrochemical measurement was conducted in simulated atmospheric corrosion solution [13].We used a cylindrical mild steel electrode pressed into a teflon holder and a platinum plate as an auxiliary electrode. To minimize the ohmic contribution, the tip of Luggin capillary was kept close to working electrode (WE). The disk end face of the mild steel electrode with 0.385 cm^2 in area served as the working surface. This enabled us to perform more exact modeling of the AC running on the metal surface in thin layers of condensed moisture. A capillary from the reference electrode was placed near the surface of the working electrode from below. Prior to processing in the VIAC vapor, the working electrode was polished and degreased with acetone. The VIAC film on the surface was preliminarily formed in vapors of the 2-propanol solution of thymol and distilled water for 24 h. The polarization investigations were performed by using a PI-50-1.1 potentiostat and a PR-8 programmer. Mild steel potential was recorded and reported *vs.* Ag/AgCl/KCl (sat.). The induced electrode potentials were recalculated relative to the normal hydrogen electrode.

The electrochemical impedance spectroscopy was measured at open circuit potential with 10 mV AC perturbation at frequency ranging from 100 kHz to 0.05 mHz with 10 points per decade. The test device and the cell configuration for the EIS measurements were the same as those for the polarization curve tests. To prove reproducibility, the polarization curve tests and the EIS measurements were repeated three times.

2.4. Surface Morphology Study (SEM)

The surface morphology and coating were examined by FEI E-SEM XL 30 (Detection of secondary electrons). For SEM images, 1 cm^2 specimen was taken.

2.5. Fourier Transformation Infrared Spectroscopic Studies (FTIR)

FTIR analys is was heald by Bruker Tensor 27 FTIR spectrometer in attenuated total reflection mode (Pike Technologies, GladiATR for FTIR with diamond crystal) and using spectral range of 4000–400 cm^{-1} with resolution of 4 cm^{-1}. The instrument was programmed to run 128 scans with the background and another 128 scans with the specimens. The registration of IR-reflectance spectra of the sample surface pretreated volatile corrosion inhibitors was performed by IR Fourier-transformed spectroscopy (Perkin Elmer) in the range of 4000–630 cm^{-1}. The registration of IR-spectra of thymol was performed on IR-Fourier-spectrometer Jasco FTIR–4000.

2.6. Theoretical Study

According to the literature data [14, 15], the adsorption activity of organic molecules and, hence, their susceptibility to chemisorption can be estimated by the reactivity indices, various electronic structure parameters obtained as a result of quantum-chemical calculations with regard for the electronic and energy characteristics of the inhibitor and the metal. Therefore, a prognostic estimate of the adsorption capacity based on the electronic characteristics of molecules such as the energy of the higher occupied molecular orbital (E_{HOMO}) and the energy of the lower vacant molecular orbital (E_{LUMO}), the energy of the molecular gap ($\Delta\varepsilon = E_{HOMO} - E_{LUMO}$) was carried out, electronegativity and chemical hardness of a molecule based on the theory of functional density. According to Koopman's theorem [16], the frontier orbital energies E_{HOMO} and E_{LUMO} are related to the ionization potential, I, and the electron affinity, A, of iron and the inhibitor molecule by the following relations: $A = -E_{LUMO}$, $I = -E_{HOMO}$.

In this adsorption, the metal acts as an electrophile while the inhibitor acts as a nucleophile. Considering the charge transfer characteristics of the adsorption, the wide use of quantum chemical calculations to study this process is justified. Calculated electron charges on the atoms of molecules were determined by their ability to chemical interaction and by the wave function of the higher occupied molecular orbital and the lower free molecular orbital, the most probable adsorption centers and the predictive adsorption capacity of the compounds were determined. In addition, it is known that the more a negative charge on a heteroatom, the better the transfer of electrons from the donor occurs. Taking into account the characteristics of the transfer of charge of adsorption, the literature substantiates the widespread use of quantum-chemical calculations for the study of this process [14, 15]. Pearson and Parr presented definitions using the finite differences method depending on electron affinity (*A*) and ionization energy (*I*) of any chemical species (atom, ion or molecule) for chemical hardness (η), and chemical potential (χ). According to the theory of functional density, the absolute electronegativity χ and chemical potential μ are the main parameters that characterize the ability of molecules to chemically interact [17-25]. Quantum chemical calculations have been performed by the HyperChem 7 [24] package. The geometry optimization was obtained by application of the restricted Hartree-Fock method (RHF) using MNDO approach with PM3 parameterization. The method of quantum chemical calculations is described in detail by Kaya *et al.* [23].

These parameters will provide insights into the mechanism of the interaction of the thymol with mild steel surface.

3. Results and Discussion

3.1. Gravimetric Measurements

The results of gravimetric investigations show that the 2-propanol solution of thymol effectively protects steel from atmospheric corrosion (Table 1). The degree of protection varies is within the range of 15.94–99.46 % depending on the concentration. Weight loss results clearly point out that on increasing the inhibitor concentration the corrosion inhibition efficiency increases while corrosion rate decreases. It should be noted that the corrosion rate decreases with increasing time of film formation. The inhibition efficiency after 72 h of thymol film-forming was higher than that after 12 and 48 h. The inhibition efficiency increases in the range of 69.55–99.87 %.

The corrosion rate and inhibition effectiveness for the thymol after 48 h film-forming were 0.0011 $g/m^2 \cdot h^1$ and 94.14 %, respectively. The protective film on the steel surface is formed for 48–50 h of its treatment with 2-propanol solution of thymol. It should be noted that the treatment of specimens in the vapor phase of individual 2-propanol does not improve the corrosion resistance of the metal.

Valuable is also the ability of the inhibitors to form stable protective films that partially retain their effect (aftereffect) even in the absence of a VCI from a corrosive medium. For this reason, we investigated the aftereffect of films formed on the metal surface after preliminary holding of the specimens in the vapor of the 2-propanol solution of thymol. It was shown (Table 3) that these films give the required aftereffect under the conditions of periodic condensation of moisture over 3% NaCl and 1N Na_2SO_4 aqueous solutions.

Table 1

Calculated corrosion rates and inhibition efficiency

Concentration inhibitor, mg/l	Corrosion rates, $g \cdot m^{-2} \cdot h^{-1}$	Inhibition efficiency (IE), %
50	0.1585	15.94
100	0.0912	51.46
200	0.0599	68.39
300	0.0382	79.67
400	0.0121	93.71
500	0.0045	97.60
600	0.0010	99.46
without inhibitor	0.1879	–

Notes: film-forming time 48 h; periodic condensation of moisture (distilled water) for 21 days

Table 2

Calculated corrosion rates and inhibition efficiency

Film-forming time, h	Corrosion rates, $g \cdot m^{-2} h^{-1}$	Inhibition efficiency (IE), %
12	0.0602	67.96
24	0.0529	71.84
40	0.0382	79.67
48	0.0011	94.14
72	0.0009	99.52
without inhibitor	0.1879	–

Notes: periodic condensation of moisture (distilled water) for 21 days; thymol concentration 600 mg/l

Table 3

Aftereffect of the films formed on St3 steel from the vapor phase of the 2-propanol solution of thymol

Testing conditions			Corrosion rate, g/(m^2·h)	Inhibition efficiency, %
Periodic moisture condensation	3% NaCl	In the vapor phase of 2-propanol solution of thymol	0.0701	80.9
		Without inhibitors	0.3663	–
	1N Na_2SO_4	In the vapor phase of 2-propanol solution of thymol	0.0198	91.6
		Without inhibitors	0.2346	–

Notes: film-forming time 48 h; experiment time 504 h

These compounds of thymol can form a protective coat to block mild steel surface. This indicates that thymol act as an inhibitor that effectively reduces the attack by the corrosive solution. The presence of the aftereffect shows that the nature of the inhibiting action is not connected with the electrostatic adsorption. It is caused by the formation of a chemisorption layer of thymol on the metal surface.

3.2. Electrochemical Measurements

The polarization measurements were performed to establish the corrosion rate determining reaction. The cathodic polarization curve recorded immediately after steel immersion in testing solution shows typical trend of oxygen reduction (Fig. 2). When analyzing the influence of VIC films on the rate of the partial electrode processes of anodic oxidation of the steel and cathodic reduction of the molecular atmospheric oxygen in 0.5M Na_2SO_4 solution with and without protective films. From the potentiodynamic polarisation curves, it can be seen that the thymol caused a decrease in both anodic and cathodic current densities, most likely due to the adsorption of the thymol at the active sites of the electrode surface.

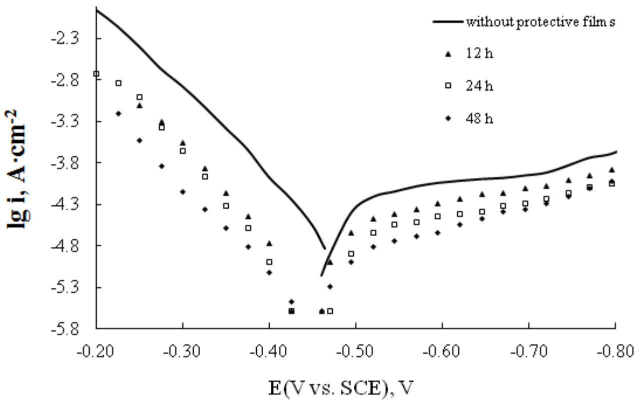


Fig. 2. Polarization curves of St3 steel in 0.5M Na_2SO_4 without protective film and with a film formed after holding for 12, 24 and 48 h in the vapor phase of the 2-propanol solution of thymol (600 mg/l)

The presence of protective film on the surface that formed in vapor phase of thymol result marked shift in the cathodic branches and to a lesser extent in the anodic branches of the polarization curves. It is also seen that all these samples shift the corrosion potential significantly to noble direction and, therefore, they are predominantly cathodic-anodic inhibitors. In other words, the inhibitor decreases the surface area for corrosion without affecting the mechanism of corrosion and only causes inactivation of a part of the metal surface.

As the time of metal treatment by the thymol increases to 48 h, the increase in the inhibiting efficiency becomes especially pronounced, this corresponds to the saturation of the surface with the inhibitor and the formation of the strongest bonds between the inhibitor and the metal. Such, a time dependence means that the formation of barrier layer on the surface is a continuous process which requires at least 48 hours.

Fig. 3 represents the Nyquist diagrams for steel in 0.5M Na_2SO_4 without protective film and with a film formed after holding for 12 and 48 h in the vapour phase of thymol. The equivalent circuit models employed for this system are presented in Fig. 4. R is a resistor (R_s – solution resistance, and R_p – charge transfer resistance), and C_{dl} represents the double layer capacitance. Since the electrochemical systems show various types of homogeneities, C_{dl} can be better substituted by a constant phase element (CPE, Q).

Table 5 gives the values of the charge transfer resistance R_s and the double layer capacitance C_{dl} obtained from the above plots. The Nyquist diagram of still in the absence of protective film describes a capacitive arc with high frequency values, which is followed by a straight line at lower frequency values. In the presence of protective film, the impedance spectrum switches to double-capacitive semicircles. It can be seen that the presence of protective film enhances the values of R_p and reduces the C_{dl} values. The decrease in C_{dl} may be due to the adsorption of thymol in the defects of the metal surface oxide layer.

Table 4

Characteristics of the polarization curves of St3 Steel in 0.5 M Na_2SO_4 after the formation of protective film from the vapor phase of the 2-propanol solution of thymol (600 mg/l)

Holding time	Currentless potential, *V*	Tafel coefficients		I_{corr}, A/cm^2 ·10^{-5}	IE, %
		b_a	b_c		
0	-0.47	0.10	0.14	13.8	–
12	-0.45	0.10	0.14	3.9	71.15
24	-0.44	0.10	0.14	2.9	81.08
48	-0.44	0.10	0.14	1.5	90.02

Table 5

Typical parameters obtained from EIS fitting results of St3 steel in 0.5M Na_2SO_4 without protective film and with a film formed after holding for 24 and 48 h in the vapour phase of thymol

Sample	Parameters obtained from EIS fitting results			
	R_s, Om·cm^2	R_p, Om·cm^2	Q, µF/cm^2	W*, Om·cm^2
Without protective films	1.26	933	0.706	–
With protective films (after 24 h film-forming)	2.01	399	0.301	–
With protective films (after 48 h film-forming)	2.99	485	0.411	

Note: **W* – resistance of Warburg, which is connected with diffusion limitation (resistance of electrolyte in pores)

The disappearance of the diffusion features in the presence of protective film indicates that the corrosion reaction is inhibited by protective film, which makes the diffusion process no longer the control process. The change in R_p values may be due to the gradual replacement of water molecules by the adsorption of the thymol molecules on the metal surface, decreasing the extent of metal dissolution reaction. The capacitance is inversely proportional to the thickness of the interface double layer. This indicates a thicker film formed after 48 h of thymol pre-treatment. The obtained results confirm the data of electrochemical polarization measurements, according to which the studied inhibitor belongs to mixed anode-cathode type with predominant cathodic control.

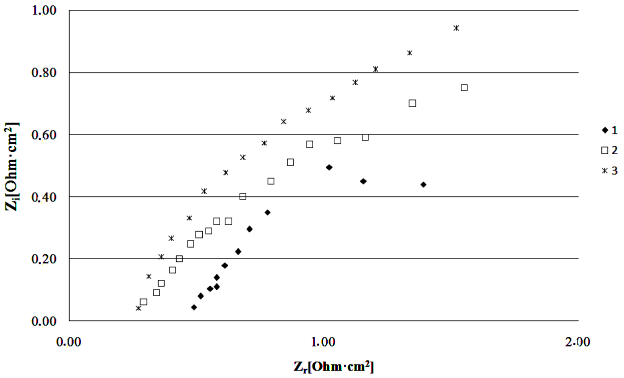


Fig. 3. Nyquist plots for a VACI under simulated atmospheric corrosion water (0.5M Na_2SO_4) layer: blank (1), after 24 h film-forming (2), and after 48 h film-forming (3)

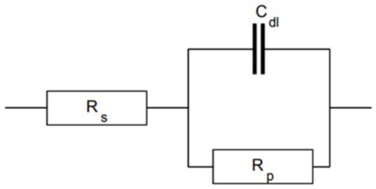
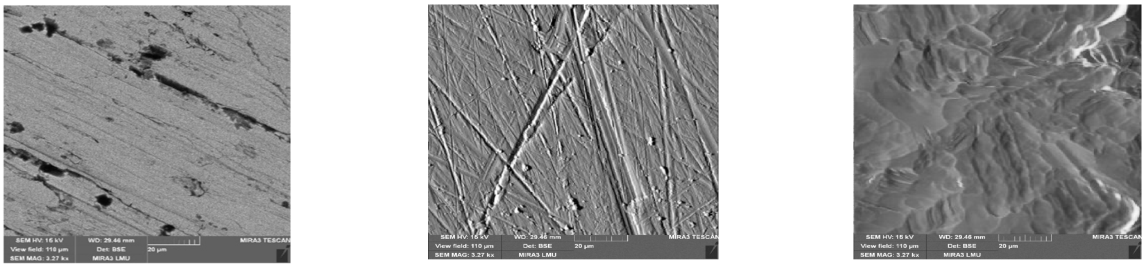


Fig. 4. Equivalent circuits for test steel

Furthermore, the inhibition efficiencies obtained from weight loss and polarization curves are in reasonably good agreement. The results obtained from weight loss and potentiodynamic polarization are in good agreement, and the compounds inhibition action could also be evidenced by surface SEM images.

3.3. SEM Surface Examination

SEM analyses were conducted in order to characterize the protective layer that formed on the low carbon steel surface. SEM images of initial surface, after 24 and 48 h for VCI film-forming are shown in Fig. 5. On the surface of the sample before exposure to volatiles of thymol there were a few scratches from the mechanical polishing treatment only (Fig. 5a). The following images (Figs. 5b,c) are of the steel surface after 24 and 48 h of exposure for the film-forming. It can be noticed that protective film looks very smooth and homogeneous at a high magnification with loosely perceptible cracks due to dehydration process that takes place in the vacuum environment necessary for SEM observations. After 48 h of film-forming the protective layer is more uniform. This improvement in surface morphology indicates the formation of a good protective film of thymol on surface.



a) b) c)

Fig. 5. SEM images of the carbon steel surface: initial surface (a); after 24 h (b); after 48 h (c) exposure for VCI film-forming

3.3. FT-Infrared Reflection Test

It is well-known that FTIR spectrophotometry is a powerful technique that can be used to determine the type of bondingof organic inhibitors absorbed on the metal surface. To establish the mechanism of forming a protective film with the surface of steel St3, the FT-IR spectrum of 2-propanol solution thymol was done (Fig. 6, *curve* a).

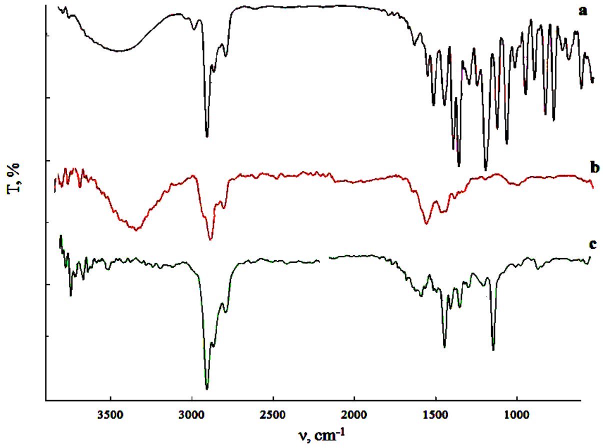


Fig. 6. FT-IR spectra of thymol (a) and after the formation of a film on mild steel for 12 h (b) and 48 h (c) in the gas-vapor atmosphere in the presence of the thymol

FT-IR spectra of the carbon steel specimens after the formation of a film for 24 and 48 h in the gas-vapor atmosphere in the presence of thymol (Fig. 6, *curves* b, c), were recorded between 500 and 4000 cm^{-1}. The obtained results indicate that after 24 h of film-forming several signals were identified that characterize the spectra of phenol and phenolic derivatives. Higher transmittance (*T*, %) was detected in case of 48 h film-forming periods. The band located at peak at 1192 cm^{-1} characteristic of polysubstituted phenolic compounds. The absorption bands at at 1498 and 1467 cm^{-1} are assigned to C–C stretching in polysubstituted aromatic rings together with the 3060–2900 cm^{-1} band. There is a sharp absorption band at the spectrum shows the signal at 1468 cm^{-}1 which can be associated with the C–C stretching vibration.

Interestingly, marked differences between 24 h and 48 h film-forming spectra in the 3100 cm^{-1} and 3650 cm^{-1} region can be noticed. The infrared spectra after 24 h film-forming, peaks at 1283, 1514, 1647, and 1064 cm^{-1} were detected for steel after 48 h treatment characteristic contributions attributed to ether bonds for phenolic derivatives [26]. It should be noted that the absorption band at 1650 cm^{-1} associated with ketone bonds, indicates a probable oxidation of the organic compound to a quinone structure.

Results demonstrated that after 24 h of film-forming protective layer includes adsorption molecules of thymol whereas after 48 h of film-forming protective layer consists of polysubstituted phenolic compounds and additionally contains ether bonds. The shielding character of the coating provides an excellent protective action to this layer inhibiting the corrosion process.

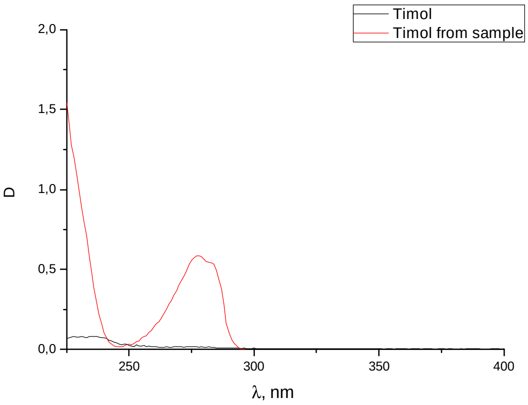


Fig. 7. Absorption spectra of 2-propanol solution of thymol and 2-propanol washouts obtained from the metal surface preliminarily treated with thymol after 48 h film-forming

To define the substances that are formed on the steel surface during exposure in inhibited phase the inhibitor layer was washed from the electrodes after 48 of exposure with 2-propanol (with a volume of 20 ml) and analysed by the spectrophotometric method (Fig. 7). Spectrum of inhibitor adsorbed on mild steel surface shows the characteristic peak. The peak is shifted, that confirms the formation of polysubstituted phenolic compounds.

3.4. Theoretical Studies of Thymol Adsorption Capacity

The molecule structure of thymol obtained after geometric optimization procedure is presented in Fig. 8. Fig. 8 shows the electric/orbital density distribution of HOMO and LUMO for thymol. The results of quantum-chemical calculations of the energy parameters of molecule are presented in Table 8.

It is found that the electron density of the frontier orbital is well proportioned. Such results indicate thymol could be both the acceptor of the electron and the donor of the electron. In other words, there is an electron transferring in the interaction between the inhibitor molecule and metal surface. Corrosion inhibition of mild steel by organic inhibitors is a complex process and is mainly influenced by charge transport. Electrophilicity, ω, is an index which measures the propensity of chemical specie to accept electrons. Thus, a good nucleophile is characterized by low values of μ and ω; whereas a good electrophile is characterized by high values of μ and ω. It is clear from Table 8 that the molecule of thymol has low electrophilicity index value and hence is a good nucleophile.


a) b)

Fig. 8. The frontier molecular orbital density distribution of thymol: HOMO (a) and LUMO (b)

Table 8

Calculated quantum chemical properties of thymol

Molecule	I	A	χ, eV	η, eV	ω, eV	$\Delta\varepsilon$	ΔE	ΔN
Thymol	9.2685	-0.2203	4.3181	4.7321	1.203	0,709	0.00023	0.26

The amount of charge transfer ΔN between the molecules and the mild steel Fe surface as calculated is given in Table 8. A positive value of ΔN indicates that the molecules act as an electron acceptor, while a negative value of ΔN indicates that the molecules act as electron donors. According to Lukovits [27], if $\Delta N < 3.6$, the molecules can be assumed to possess charge transfer ability towards the metal surface.

4. Conclusions

In this study, it was shown that the thymol is effective corrosion inhibitor for temporary protection of mild steel. Potentiodynamic polarization parameters reveal that the inhibitor affects both anodic and cathodic reactions and acts more or less as a mixed inhibitor. It is shown that the inhibition of the atmospheric corrosion of steels after treatment in the vapor of volatile compound of thymol, occurs due to the blocking of the metal surface by polysubstituted phenolic compounds. Morphological studies supported the formation of a protective layer on the surfaces. The formation of a film with maximum protective characteristics is completed after holding of St3 steel for 48 h in the vapor of volatile compounds of 2-propanol solution thymol. It is characterized by the aftereffect under the conditions of periodic condensation of moisture over a 3% NaCl and, in 1N Na_2SO_4.

References

[1] Zhang D-Q., Gao L-X., Zhou G-D.: Surf. Coat. Technol., 2010, **204**, 1646. https://doi.org/10.1016/j.surfcoat.2009.10.054
[2] Zhang D-Q., An Z-X., Pan Q-Y. *et al.*: Corros. Sci., 2006, **48**, 1437. https://doi.org/10.1016/j.corsci.2005.06.007

[3] Sudheer A., Quraishi E., Eno E., Natesan M.: Int. J. Electrochem. Sci., 2012, **7**, 7463.
[4] Quraishi M., Jamal D.: Corrosion, 2002, **58**, 5, 387. https://doi.org/10.5006/1.3277627
[5] Montemor M.: Act. Protect. Coat., 2016, **233**, 107. https://doi.org/10.1007/978-94-017-7540-3_6
[6] Chygyrynets' E., Vorobyova V.: Chem. Chem. Technol., 2014, **8**, 235.
[7] Vorob'iova V., Chyhyrynets' O., Vasyl'kevych O.: Mater. Sci., 2015, **50**, 726. https://doi.org/10.1007/s11003-015-9778-z
[8] Chyhyrynets O.,Vorob'iova V.: Mater. Sci., 2013, **49**, 318. https://doi.org/10.1007/s11003-013-9617-z
[9] Poongothai N., Rajendran P., Natesan M. *et al.*: Indian J. Chem. Technol., 2005, **12**, 641.
[10] Premkumar P., Kannan K., Natesan M.: Asian J. Chem., 2008, **20**, 445.
[11] Premkumar P., Kannan K., Natesan M.: J. Metall. Mater. Sci., 2008, **50**, 227.
[12] Li X., Deng S., Fu H., Xie X.: Corros. Sci., 2014, **78**, 29. https://doi.org/10.1016/j.corsci.2013.08.025
[13] Leygraf C., Wallinder I.,Tidblad J., Graedel T.: Atmospheric Corrosion. John Wiley & Sons, Inc., Hoboken 2016.
[14] Kaya S., Tüzün B., Kaya C., Obot I.: J. Taiwan Inst. Chem. Eng., 2016, **58**, 528. https://doi.org/10.1016/j.jtice.2015.06.009
[15] Gece G.: Corros. Sci., 2008, **50**, 11, 2981. https://doi.org/10.1016/j.jtice.2015.06.009
[16] Koopmans T.: Physica, 1934, **1**, 104. https://doi.org/10.1016/S0031-8914(34)90011-2
[17] Kovacevic N., Kokalj A.: Corros. Sci., 2011, **53**, 3, 909. https://doi.org/10.1016/j.corsci.2010.11.016
[18] Parr R., Pearson R.: J. Am. Chem. Soc., 1983, **105**, 7512. https://doi.org/10.1021/ja00364a005
[19] Parr R., Donnelly R., Lewy M., Palke W.: J. Chem. Phys., 1978, **68**, 3801. https://doi.org/10.1063/1.436185
[20] Pearson R.: Proc. Nats. Acad. Sci. USA, 1986, **83,** 8440.
[21] Chattaraj P., Sarkar R., Roy D.: Chem. Rev., 2006, **106**, 2065. https://doi.org/10.1021/cr040109f
[22] Parr R., von Szentpaly L., Liu S.: J. Am. Chem. Soc. 1999, **121**, 1922. https://doi.org/10.1021/ja983494x
[23] Kaya S., Kaya C.: Comput. Theor. Chem., 2015, **1052**, 42. https://doi.org/10.1016/j.comptc.2014.11.017
[24] HyperChemTM, Hypercube, Inc., 1994
[25] Rosliza R. *et al.*: J. Appl. Electrochem., 2010, 4**0**, 833. https://doi.org/10.1007/s10800-009-0066-1
[26] Ferreira M., Varela H., Torresi R., Tremiliosi-Filho G.: Electrochim. Acta, 2006, **52**, 434. https://doi.org/10.1016/j.electacta.2006.05.025
[27] Lukovits I., Kálmán E., Zucchi F.: Corrosion. 2001, **57**, 3. https://doi.org/10.5006/1.3290328

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ЕКСПЕРИМЕНТАЛЬНІ ТА ТЕОРЕТИЧНІ ДОСЛІДЖЕННЯ ПРОТИКОРОЗІЙНИХ ВЛАСТИВОСТЕЙ ТИМОЛУ

Анотація. *Тимол досліджено як новий леткий інгібітор атмосферної корозії сталі. Для оцінки складу та характеристики сформованих захисних шарів використовували гравіметричні та електрохімічні дослідження, доповнені спектральними FT-IR та мікроскопічними методами аналізу SEM. Плівка, утворена на поверхні сталі з парогазової фази тимолу, забезпечує ефект післядії на рівні 90% за періодичної конденсації вологи впродовж 504 годин. Для оцінки адсорбційної здатності тимолу проведені квантово-хімічні розрахунки енергетичних параметрів молекули тимолу.*

Ключові слова: *атмосферна корозія, тимол, сталь, інгібітор корозії, квантово-хімічні розрахунки.*