THE ROLE OF SURFACE HYDROPHOBIZATION OF MILD STEEL BY SOME TRIAZOLE DERIVATIVES IN ACIDIC MEDIUM

PlotnikovaM.D., Shcherban’M.G., SheinA.B., ShitoevaA.D.
Perm State University

Corrosion is a widely studied field of science. In order to understand mechanisms of action of corrosion inhibitors, the reactions at the interfaces between the corrosive electrolyte and a steel surface are investigated. Naturally, these reactions are strongly affected by the nature and properties of the steel surfaces, but the interaction between steel surface and the molecules of inhibitor plays important role. The aim of this work is to confirm the assumption about the formation of a protective film and the chemical adsorption of some triazole derivatives on mild steel surfaceby physicochemical methods.

The tested inhibitors, namely 4,5-diphenyl-4H-1,2,4-triazole-3-thiol (4,5-PhTAT) and 3,4-diphenyl-5-(prop-2-yn-1-ylthio)-4H-1,2,4-triazole (3,4-PhPTTA), were synthesized according to a previously described experimental procedure [1, 2].

Potentiodynamic polarization measurements were carried out using electrochemical analytical system (Solatron 1280 C). On the basis of Young’s equation plus Owen-Wendt’s theory, the surface free energies of steel surface can be calculated using the contact angles between the two test liquids (water and diethylene glycol) and steel surface [3]. Mild steel St3 has been used for all measurements.

Polarization curves for mild steel in 0.1 N H_2SO_4 solution without and with addition of 100 mg/l of 4,5-PhTAT and 3,4-PhPTTA are shown in Fig. 1.

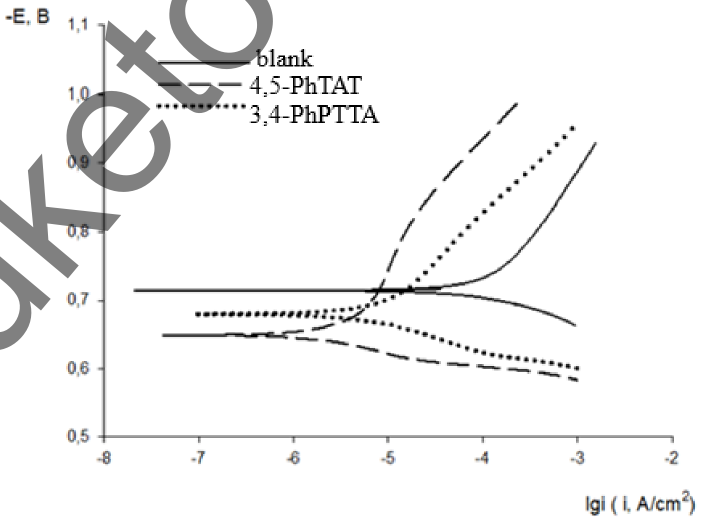

Figure 1. Potentiodynamic polarization curves for mild steel in 0.1 N H_2SO_4 with different triazole derivatives.

The presence of both triazoles resulted in a shift of the corrosion potential towards the anodic direction in comparison with the result obtained in the blank acid solution. The anodic and the cathodic current densities were decreased, indicating that 4,5-PhTAT and 3,4-PhPTTA suppressed both the anodic and cathodic reactions.

The calculation of the free surface energy (SFE) of steel was carried out before and after contact with a corrosive medium toconfirm the assumptions about the formation of the protective film and the chemical nature of adsorption. The value of SFE due to the isolation of its polar (γ^p) and dispersion (γ^d) components can indicate the direction of further modification to increase resistance of the corrosion system.

The immersion of the samples into blank sulfuric acid leads to significant hydrophobization of the steel surface, the contact angle increases to 136° as a result of the dissolution of iron and the surface enrichment with carbon. [4, 5].

The steel surface in the presence of an inhibitor is also hydrophobized – the contact angles are in the range of 105° – 130°. Probably, the effect of hydrophobization of the surface is associated with the formation of a protective film of the inhibitor, and not with the increase of the carbon concentration on the steel surface.

Also the ratio of the polar and dispersion components of the free surface energy changes when samples are kept in inhibited acid. Calculated values SFE are presented in Table 1. Also in Table 1 the degrees of protection calculated from the results of weight loss testing are presented.

Table 1. – Surface energies for test liquids (22 °C) and degree of protection of St3 after weight loss tests in the presence of triazole derivatives in 0.1 N H_2SO_4 solution

Conc., mg/l	γ^p_{LG}, mJ/m^2	γ^d_{LG}, mJ/m^2	γ_{LG}, mJ/m^2	$\gamma^d_{LG}/\gamma^p_{LG}$	Z, %
Before immersion	6,2	24,98	31,18	4,0	
0	43,4	149,96	193,32	3,5	
4,5-PhTAT					
50	3,73	70,19	73,92	18,8	96
100	6,40	78,18	84,58	12,2	92
200	9,25	83,96	93,21	9,1	92
3,4-PhPTTA					
50	1,13	53,40	54,53	47,3	94
100	1,06	42,12	43,18	39,7	95
200	2,53	43,28	45,82	17,3	95

From this Table, we can see that after weight loss testing in an uninhibited solution of 0.1 N H_2SO_4, the ratio of the dispersion and polar components of the free surface energy changed slightly.The addition of the inhibitor increased in the dispersion component relative to the polar one. The increase is probably caused by the formation of hydrophobic adsorption layer on the surface blocking interaction between the steel surface and corrosion medium.

Since the corrosion rate depends on the contact area of steel with the corrosion medium, the degree of protection of the inhibitors is the higher, the more dispersion component of the free surface energy. Thus hydrophobization of the surface has a positive effect on the inhibition efficiency, as evidenced by the growth of the dispersion component of SFE.

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COMPUTATIONAL STUDY OF LUPININ AND ITS DERIVATIVES FOR DIHYDROFOLATE REDUCTASE INHIBITION

Pustolaikina I.A.[1],Fazylov S.D.[2], Nurmaganbetov Z.S.[2],
Normatov S.Sh. [1], KimV.V. [1]

[1]Karagandy University named after E.A.Buketov, Karaganda, 100024, Kazakhstan
[2]Institute of Organic Synthesis and Coal Chemistry, Karaganda, 100008, Kazakhstan

The quinolizidine alkaloid lupinine (Figure 1) was chemically modified at theInstitute of Organic Synthesis and Coal Chemistry (Karaganda, Kazakhstan). As a result, more than 25 of lupinine new derivatives were obtained [1-3].Antibacterial properties were established for the synthesized substances by the *in vitro* method. The aim of this study was to evaluate *in silico* the dihydrofolate reductase (Figure 2) inhibitory potential for the 7 most promising lupinine derivatives using the molecular docking method.