

A Density Functional Theory (DFT) based Analysis on the Inhibition Performances of Some Triazole Derivatives for Iron Corrosion

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ABSTRACT

Iron is one of the widely used metals in industry. For that reason, the prevention of the corrosion of such metals via new designed inhibitor systems is among the interest of corrosion scientists. In the present paper, we investigated the corrosion inhibition performance of 2-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl) methoxy) benzaldehyde (A), 4-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl) methoxy) benzaldehyde (B), 4-((4-nitrophenoxy) methyl)-1-(4-nitrophenyl)-1H-1,2,3-triazole (C), 4-methyl-7-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl) methoxy)-2H-chromen-2-one (D) against iron corrosion. For the mentioned inhibitor systems, important reactivity descriptors like frontier orbital energies, chemical potential, electronegativity, hardness, softness, polarizability, dipole moment, back-donation energy, electrophilicity, electroaccepting power and electrodonating power were calculated and discussed. Calculations were repeated using various methods and basis sets in different phases. The chemical reactivities of the inhibitors were predicted in the light of well-known electronic structure rules like Maximum Hardness and Minimum Polarizability Principles. The obtained data showed that the best corrosion inhibitor among them is molecule D while the most stable molecule is molecule C. The theoretical data support the experimental observations.

Keywords: DFT, Electronic Structure, Corrosion inhibitor, Thiazole derivatives.^ankarakus@cumhuriyet.edu.tr^{ib} <https://orcid.org/0000-0001-6223-7669>^b savaskaya@cumhuriyet.edu.tr ^{id} <https://orcid.org/0000-0002-0765-9751>

Introduction

Corrosion can be defined as natural process converting the metals to their sulfides, oxides and hydroxides [1,2]. Adding the inhibitor molecules to corrosive media, the prevention of the corrosion of metals is among the interests of corrosion scientists. The molecules acting as effective corrosion inhibitors are easily adsorbed on metal surfaces through an electron transfer between inhibitor and metal surface. Many theoretical and experimental corrosion scientists reported the high inhibition performance of π -systems and heterocyclic compounds including especially heteroatoms like nitrogen, sulfur and oxygen [3,4]. It is well-known that a triazole is a heterocyclic molecule including a five membered ring with two carbons and three nitrogens. Triazole's closed molecular formula is $C_2H_3N_3$. Some important papers about the high effectiveness of triazole derivatives against the corrosion of various metal and alloys are available in the literature. M. M. Abdelsalem and coworkers [5] synthesized three triazole derivatives, namely -((1H-1,2,4-triazol-3-ylimino) methyl)naphthalen-2-ol (TMN), N-(furan-2-ylmethylene)-1H-1,2,4-triazol-3-amine (FTA) and N-(thiophen-2-ylmethylene)-1H-1,2,4-triazol-3-amine (TTA) with the help of ultrasonic irradiation and investigated their corrosion inhibition performances. In the analysis made via some experimental and theoretical tools, corrosion inhibition efficiency ranking obtained for steel was reported as: TMN> TTA>FTA. In another paper penned

by Belghiti and coworkers [6] analyzed the corrosion inhibition performance of four triazole derivative in strong phosphoric acid medium for steel. This study was also a proof of which triazole derivatives are effective corrosion inhibitors against the corrosion of metals and alloys.

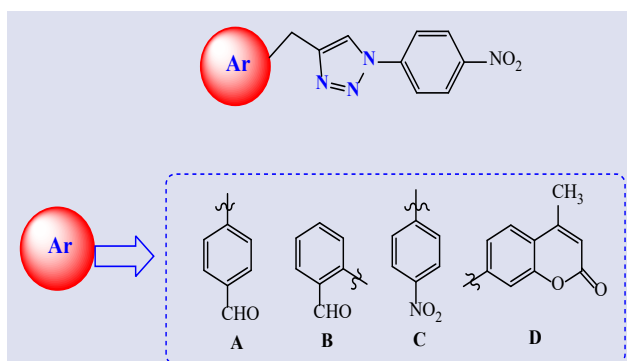


Figure 1. Molecular structures of the inhibitor systems considered in this study.

In a recent paper published by Jaber and coworkers [7], four new triazole derivatives were synthesized via regioselective click reaction and investigated their corrosion inhibition performances using only experimental procedures. The molecular structures of the mentioned triazole derivatives are presented in Fig.

1. The aim of this article is to theoretically analyze the corrosion inhibition performances of molecules A, B, C and D and is to predict their chemical reactivities through the some electronic structure rules. The obtained theoretical data will be helpful to experimental corrosion scientists in the design of new triazole derivatives.

Computational Details and Equations

Conceptual Density Functional Theory (CDFT) can be considered as the reactivity related branch of DFT. CDFT includes many simple formulae to compute the quantum chemical descriptors and well-known electronic structure rules based on these descriptors. In CDFT, the following mathematical relations for chemical potential (μ), electronegativity (χ), hardness (η) and softness (σ) are presented [8,9].

$$\mu = -\chi = \left[\frac{\partial E}{\partial N} \right]_{v(r)} \quad (1)$$

$$\eta = \left[\frac{\partial^2 E}{\partial N^2} \right]_{v(r)} \quad (2)$$

$$\sigma = 1 / \eta \quad (3)$$

Here, E and N represents the total electronic energy and total number of the electrons of any chemical system, respectively. If one applies the finite differences approach to the mathematical relations given above, for the calculation of the aforementioned quantum chemical descriptors, the following simple formulae based on ground state ionization energy (I) and ground state electron affinity (A) of atoms, ions and molecules are obtained [10].

$$\mu = -\chi = -\left(\frac{I + A}{2} \right) \quad (4)$$

$$\eta = I - A \quad (5)$$

First electrophilicity index (ω_1) mathematically introduced by Parr, Szentpaly and Liu [11] is calculated based on absolute hardness and absolute electronegativities of the chemical systems via the equation given below

$$\omega_1 \equiv \chi^2 / 2\eta \quad (6)$$

Second electrophilicity index that its usefulness is emphasized by especially Szentpaly and Kaya [12] is calculated as:

$$\omega_2 = I.A / I - A \quad (7)$$

Electroaccepting power (ω^+) and electrodonating power (ω^-) parameters introduced by Gazquez and coworkers [13] in 2007 are calculated from the following equations. These parameters depending on ionization energy and electron affinity of atom, ions and molecules like other Conceptual DFT based descriptors are widely used in corrosion science.

$$\omega^+ = (I + 3A)^2 / (16(I - A)) \quad (8)$$

$$\omega^- = (3I + A)^2 / (16(I - A)) \quad (9)$$

Back-donation energy (ΔE_{b-d}) is closely related to the absolute hardness of a chemical system and is calculated from the following equation

$$\Delta E_{b-d} = -\frac{\eta}{4} \quad (10)$$

In the corrosion science, to compute the fraction of the electrons transferred from inhibitor to metal surface and metal-inhibitor interaction energy, the following equations are used.

$$\Delta N = \frac{\phi_{Fe} - \chi_{inh}}{2(\eta_{Fe} + \eta_{inh})} \quad (11)$$

$$\Delta \psi = -\frac{(\phi_{Fe} - \chi_{inh})^2}{4(\eta_{Fe} + \eta_{inh})} \quad (12)$$

In these equations, ϕ_{Fe} is work function computed for Fe (110) surface and its numerical value is 4.82 eV. Chemical hardness of Fe surface is taken as $\eta_{Fe}=0$ because $I=A$ for a bulk. In the equations χ_{inh} and η_{inh} represent the electronegativity and chemical hardness of inhibitor molecule, respectively [15].

Gas phase calculations were performed using HF, B3LYP and M062X methods and considering 6-31++G(d,p), SDD, 6-311++G(d,p) basis sets. In the calculations in water phase, only B3LYP method was preferred. Since the corrosion process is generally carried out in aqueous environments, it is essential to make the calculations also in the aqueous phase. For this reason, we performed the PCM (polarisable continuum model) method to investigate the solvent effect of water. In the prediction of ionization energy and electron affinities of the studied inhibitor molecules, we considered Koopmans Theorem [16] giving the following relations based on HOMO and LUMO orbital energies.

$$I = -E_{HOMO} \quad (13)$$

$$A = -E_{LUMO} \quad (14)$$

Results and Discussion

In this paper, using Conceptual Density Functional Theory based chemical reactivity parameters and electronic structure rules, we investigated the corrosion inhibition performances of some triazole derivatives against the corrosion of the iron. For this goal, well-known parameters like hardness, electrophilicity, electronegativity, back-donation energy, polarizability, metal-inhibitor interaction energy, electrodonating/accepting powers were computed and their relation with electron donating ability of molecules were discussed in detail. In Table 1, computed quantum chemical parameters for studied inhibitor molecules in the gas phase while Table 2 reflects the results obtained in aqueous media. Fig. 2 visually presents optimized structures, HOMOs, LUMOs and ESP maps obtained at B3LYP/6-311++g (d p) calculation level of the studied molecular systems. The different values in the electrostatic potential maps (ESP) are presented through different colors. In these maps, red color presents the region of the most negative electrostatic potential, blue color stands for the region of the most positive electrostatic potential and green color stands for the region of the zero electrostatic potential. The reddest region is the region most suitable for protonation

Molecular Orbital Theory widely uses the HOMO and LUMO energies to explain the acidic and basic behaviour of the molecules. It should be noted that the molecules with high value of HOMO energy acts as effective corrosion inhibitors because they give the electrons easily to metals and alloys. Additionally, the molecular systems with low values of LUMO energy are good electron acceptors. According to computed HOMO and LUMO orbital energies, the corrosion inhibition efficiency order of the studied molecules can be given as: D>B>A>C. Chemical hardness [17] is a powerful tool to explain the stability of molecules as a good measure of the chemical reactivity because this quantity represents the resistance towards electron cloud polarization of atomic and molecular systems. According to Maximum Hardness Principle [18], it can be noted that hard chemical systems exhibits high stability and cannot show high efficiency against the corrosion of metal surfaces. Considering the inverse relation between hardness and polarizability, it can be said with ease that the molecular systems with high polarization are effective corrosion inhibitor [19]. As can be seen from the computational details section, back-donation energy is closely related to the chemical hardness of molecules.

Table 1. Calculated quantum chemical parameters for studied inhibitor molecules in the gas phase

Molecule	E_{HOMO}	E_{LUMO}	χ	η	ω_1	ω_2	$\Delta E_{\text{b-d}}$	ω^-	ω^+	α (au)
B3LYP/6-31++G (d, p)										
A	-7.046	-3.260	5.153	3.786	3.507	6.067	-0.947	9.827	4.674	245.542
B	-7.029	-3.302	5.166	3.727	3.580	6.227	-0.932	9.975	4.809	251.926
C	-7.423	-3.355	5.389	4.068	3.569	6.122	-1.017	10.088	4.699	253.456
D	-6.650	-3.260	4.955	3.39	3.621	6.395	-0.848	9.932	4.977	295.346
B3LYP/SDD										
A	-7.080	-3.535	5.308	3.545	3.973	7.060	-0.886	10.822	5.514	221.750
B	-7.042	-3.574	5.308	3.468	4.062	7.257	-0.867	10.995	5.687	228.346
C	-7.514	-3.638	5.576	3.876	4.011	7.053	-0.969	11.052	5.476	232.081
D	-6.734	-3.530	5.132	3.204	4.110	7.419	-0.801	10.986	5.854	270.050
B3LYP/6-311++G (d, p)										
A	-7.092	-3.255	5.174	3.837	3.488	6.016	-0.959	9.802	4.629	244.061
B	-7.076	-3.295	5.186	3.781	3.556	6.166	-0.945	9.941	4.755	250.424
C	-7.468	-3.348	5.408	4.12	3.549	6.069	-1.030	10.060	4.652	251.479
D	-6.693	-3.253	4.973	3.44	3.595	6.329	-0.860	9.891	4.918	294.058
HF/6-31++G (d, p)										
A	-9.302	0.685	4.309	9.987	0.929	-0.638	-2.497	4.637	0.329	214.386
B	-9.263	0.662	4.301	9.925	0.932	-0.618	-2.481	4.634	0.333	217.548
C	-9.842	0.599	4.622	10.441	1.023	-0.565	-2.610	5.009	0.387	217.744
D	-8.785	0.699	4.043	9.484	0.862	-0.647	-2.371	4.338	0.295	255.031
HF/SDD										
A	-9.577	0.204	4.687	9.781	1.123	-0.200	-2.445	5.200	0.514	194.892
B	-9.513	0.188	4.663	9.701	1.120	-0.184	-2.425	5.178	0.516	198.034
C	-10.200	0.111	5.045	10.311	1.234	-0.110	-2.578	5.635	0.590	200.356
D	-9.097	0.224	4.437	9.321	1.056	-0.219	-2.330	4.912	0.476	234.639
HF/6-311++G (d, p)										
A	-9.324	0.712	4.306	10.036	0.924	-0.661	-2.509	4.628	0.322	214.850
B	-9.287	0.635	4.326	9.922	0.943	-0.594	-2.481	4.669	0.343	274.138
C	-9.866	0.577	4.645	10.443	1.033	-0.545	-2.611	5.041	0.396	217.927
D	-8.800	0.709	4.046	9.509	0.861	-0.656	-2.377	4.338	0.293	255.792
M062X/6-31++G (d, p)										
A	-8.355	-2.098	5.227	6.257	2.183	2.801	-1.564	7.370	2.144	231.889
B	-8.313	-2.128	5.221	6.185	2.203	2.860	-1.546	7.403	2.183	236.737
C	-8.753	-2.185	5.469	6.568	2.277	2.912	-1.642	7.699	2.230	237.164
D	-7.898	-2.094	4.996	5.804	2.150	2.849	-1.451	7.161	2.165	278.454
M062X/SDD										
A	-8.519	-2.491	5.505	6.028	2.514	3.520	-1.507	8.157	2.652	209.602
B	-8.459	-2.517	5.488	5.942	2.534	3.583	-1.486	8.184	2.696	214.384
C	-8.998	-2.585	5.792	6.413	2.615	3.627	-1.603	8.527	2.735	217.044
D	-8.108	-2.480	5.294	5.628	2.490	3.573	-1.407	7.979	2.685	254.286
M062X/6-311++G (d, p)										
A	-8.413	-2.106	5.260	6.307	2.193	2.809	-1.577	7.410	2.150	230.562
B	-8.373	-2.136	5.255	6.237	2.213	2.868	-1.559	7.444	2.189	235.462
C	-8.821	-2.194	5.508	6.627	2.289	2.920	-1.657	7.745	2.238	235.753
D	-7.951	-2.101	5.026	5.85	2.159	2.856	-1.463	7.197	2.171	277.196

So, it is not difficult to predict that the molecules with more negative values of the back-donation energy are not effective corrosion inhibitors. In the light of computed hardness, polarizability and back-donation energy data, the corrosion inhibition efficiency order can be given as: D>B>A>C. Electronegativity [20,21] is among key parameters used to explain the nature of the chemical interactions and chemical bonding. Shortly, it can be defined as the electron withdrawal powers of atoms, ions and molecules. In the light of this definition, it is clear that effective corrosion inhibitors should not have high electronegativity values. Computed electronegativity values also imply the high efficiency of molecule D. According to Minimum Electrophilicity Principle, in stable states and conformers, electrophilicity is minimized. Normally, in corrosion inhibition studies that don't consider the Minimum Electrophilicity Principle, it is noted that the molecules with high value of electrophilicity index cannot act

effective corrosion inhibitors. On the other hand, Minimum Electrophilicity Principle implies that the molecules with large value of electrophilicity index are more reactive than others. Our results support the Minimum Electrophilicity Principle and this principle predicts the best corrosion inhibitor as molecule D. Electrodonating power and electroaccepting power are among the parameters used in corrosion inhibition prediction. Good corrosion inhibitors have high value of electrodonating power and low value of electroaccepting power. The experimentally obtained corrosion inhibition efficiency ranking for the studied inhibitor systems is the same of the ranking obtained with the help of Conceptual Density Functional Theory based theoretical analyses. Chemical reactivity analysis made here will assist experimental chemists in the synthesis or design of more reactive or more stable Triazole derivatives.

Table 2. Calculated quantum chemical parameters for studied inhibitor molecules in the aqueous phase

Molecule	E_{HOMO}	E_{LUMO}	χ	η	ω_1	ω_2	ΔE_{b-d}	ω^-	ω^+	α (au)
B3LYP/6-311++G (d, p)										
A	-6.778	-3.279	5.0285	3.499	3.613	6.352	-0.8748	9.960	4.931	331.174
B	-6.853	-3.266	5.0595	3.587	3.568	6.240	-0.8968	9.890	4.831	335.582
C	-7.080	-3.284	5.182	3.796	3.537	6.125	-0.9490	9.902	4.720	343.462
D	-6.489	-3.278	4.8835	3.211	3.714	6.624	-0.8028	10.070	5.186	398.115
HF/6-311++G (d, p)										
A	-9.082	0.818	4.132	9.9	0.862	-0.750	-2.4750	4.409	0.277	283.113
B	-9.072	0.819	4.1265	9.891	0.861	-0.751	-2.4728	4.403	0.277	284.948
C	-9.507	0.817	4.345	10.324	0.914	-0.752	-2.5810	4.646	0.301	286.180
D	-8.640	0.822	3.909	9.462	0.807	-0.751	-2.3655	4.161	0.252	335.839
M062X/6-311++G (d, p)										
A	-8.193	-2.074	5.1335	6.119	2.153	2.777	-1.5298	7.256	2.122	307.319
B	-8.181	-2.074	5.1275	6.107	2.153	2.778	-1.5268	7.251	2.123	311.069
C	-8.494	-2.076	5.285	6.418	2.176	2.748	-1.6045	7.396	2.111	313.699
D	-7.814	-2.073	4.9435	5.741	2.128	2.822	-1.4353	7.087	2.144	368.684
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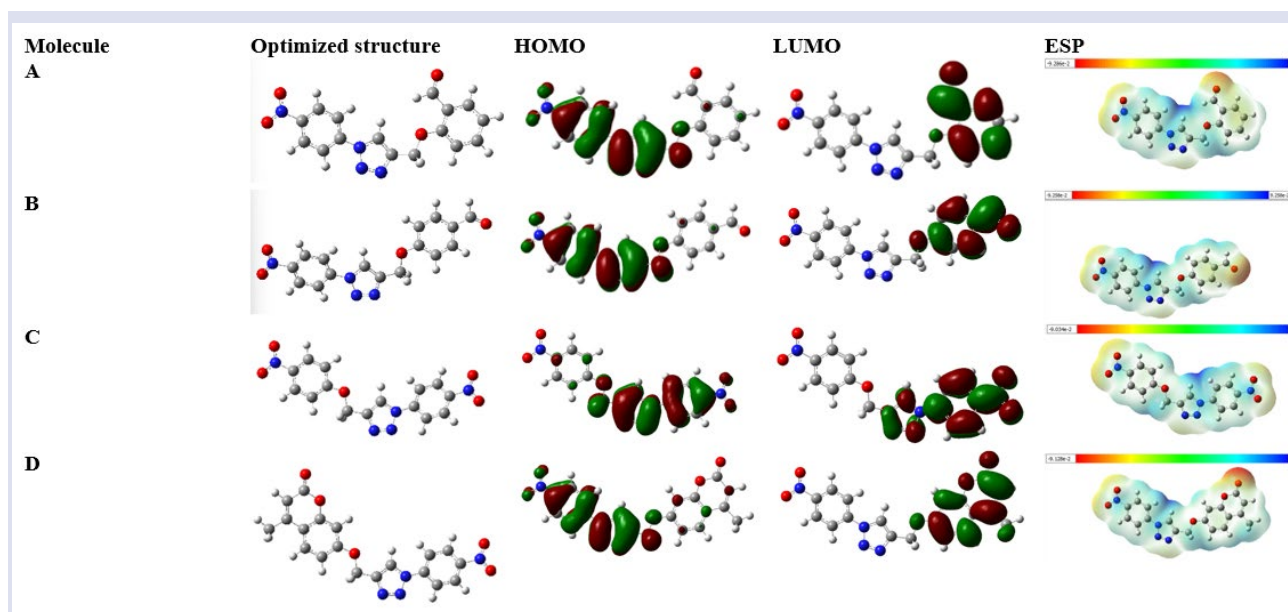


Figure 2. Optimized structures, HOMOs, LUMOs and ESP maps obtained at B3LYP/6-311++g (d p) calculation level of the studied molecular systems.

Conclusion

The present paper includes detailed Conceptual Density Functional Theory based computations to predict the corrosion inhibition performances of some triazole derivatives, namely, 2-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl) methoxy) benzaldehyde (A), 4-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl) methoxy) benzaldehyde (B), 4-((4-nitrophenoxy) methyl)-1-(4-nitrophenyl)-1H-1,2,3-triazole (C), 4-methyl-7-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl) methoxy)-2H-chromen-2-one (D). According to obtained data in both gas phase and aqueous phase, the best corrosion inhibitor among studied molecules is molecule D. Theoretical analyzes made are in good agreement with experimental observations and the predictions done in the light of popular electronic structure rules like Minimum Polarizability, Minimum Electrophilicity and Maximum Hardness Principles. The calculations and structural analyses made will be helpful for experimentalists in the design and synthesis of new triazole derivatives as corrosion inhibitor.

Conflicts of Interest

There are no conflicts of interest in this work.

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